

NUMERICAL STUDY OF ANISOTROPIC IRREVERSIBLE DEPOSITION OF EXTENDED OBJECTS ON A TRIANGULAR LATTICE

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Abstract

The properties of the anisotropic random sequential adsorption (RSA) of objects of various shapes on a two-dimensional triangular lattice are studied numerically by means of Monte Carlo simulations. The depositing objects are formed by self-avoiding lattice steps. Anisotropy is introduced by positing unequal probabilities for orientation of depositing objects along different directions of the lattice. This probability is equal p or $(1 - p)/2$, depending on whether the randomly chosen orientation is horizontal or not, respectively. Approach of the coverage $\theta(t)$ to the jamming limit θ_{jam} is found to be exponential $\theta_{jam} - \theta(t) \propto \exp(-t/\sigma)$, for all probabilities. It was shown that the relaxation time σ increases with the degree of anisotropy in the case of elongated and asymmetrical shapes. However, for rounded and symmetrical shapes, values of σ and θ_{jam} are not affected by the presence of anisotropy.

Introduction

Deposition, or adsorption, of extended objects at different surfaces is of considerable interest for a wide range of applications in biology, nanotechnology, device physics, physical chemistry, and materials science [1,2]. Theoretically, several models have been developed to capture the basic physics of this situation, and by far the most studied is that of random sequential adsorption (RSA) [3]. In this model particles (objects) are sequentially deposited on the randomly chosen site of the substrate. When deposited, such objects are irreversibly attached to the site. If the chosen site is already occupied, the deposition is rejected, the particle is discarded, and the deposition is next attempted at a different randomly chosen site. For lattice models the approach of the coverage fraction to its jamming limit is given by the time dependence:

$$\theta(t) \sim \theta_{jam} - \Delta\theta \exp(-t/\sigma), \quad (1)$$

where parameters θ_{jam} , $\Delta\theta$, and σ depend on the shape and orientational freedom of depositing objects [4,5].

In order to account for inhomogeneous surfaces in our RSA model, we have introduced anisotropy in the deposition procedure. Namely, even when the deposition at a randomly chosen site is allowed, the probability for deposition is different along different directions of the underlying lattice. This simple modification introduces preferential direction in the deposition process and, depending on the shape of deposited objects, imposes this specific “patterning” on the deposited layer.

The main goal of the present study is to investigate the interplay between the anisotropy of deposition and the symmetry properties of deposited shapes. This work discusses the rapidity of the approach to the jamming state and the values of the jamming coverages for various degrees of anisotropy of the deposition process. Here we focus our interest on the influence of the order of symmetry axis of the shape on the kinetics of the deposition processes under anisotropic conditions.

Simulation method

The depositing shapes are modeled by directed self-avoiding walks on a triangular lattice. Examples of such walks for $l = 1, 2$, and 6 are shown in Table I. At each Monte Carlo step we randomly select a lattice site and try to deposit the shape of length l . If the selected site is occupied by a deposited object, the adsorption attempt is rejected. If the selected site is unoccupied, we fix the beginning of the walk that makes the chosen shape at this site.






(x)	shape	n_s	ℓ
(A)		2	1
(B)		2	2
(C)		1	2
(D)		3	3
(E)		6	6

Table I. Various shapes (x) of length l on a triangular lattice. n_s denotes the order of symmetry axis of the shape.

Anisotropy is introduced by positing unequal rates for deposition of objects in the three possible directions. The choice of the horizontal direction occurs with probability p and for each of the other two directions with probability $(1 - p)/2$. Hence, the value of $p = 1/3$ corresponds to the isotropic case. We randomly pick one of the six possible orientations with a corresponding probability, start the l -step walk in that direction, and search whether all successive l sites are unoccupied. If so, we occupy these $l + 1$ sites and deposit the object; otherwise, the deposition attempt is rejected.

The Monte Carlo simulations are performed on a 2D triangular lattice of size $L = 128$. The time is counted by the number of attempts to select a lattice site and scaled by the total number of lattice sites. Periodic boundary conditions are used in all directions. The data are averaged over 1000 independent runs for each depositing object. The finite-size effects, which are generally weak, can be neglected for object sizes $< L/8$.

Results and discussion

We study the anisotropic irreversible deposition of objects of various shapes (Table I). In the case of isotropic deposition ($p = 1/3$), according to parameter σ (Eq.(1)), all extended shapes can be divided into four groups:

- (a) Shapes with asymmetry axis of first order, $n_s = 1$, with $\sigma \simeq 5.9$
- (b) Shapes with a symmetry axis of second order, $n_s = 2$, with $\sigma \simeq 3.0$
- (c) Shapes with a symmetry axis of third order, $n_s = 3$, with $\sigma \simeq 2.0$
- (d) Shapes with a symmetry axis of sixth order, $n_s = 6$, with $\sigma \simeq 0.99$.

This means that at late enough times, the rotational symmetries associated with specific shapes have a substantial influence on the adsorption rate of the objects. More symmetric shapes reach their jamming coverage faster; i.e., the relaxation time σ is smaller for more symmetric objects. At large times, adsorption events take place on the islands of unoccupied sites. The individual islands act as selective targets for specific deposition events. In other words, there is only a restricted number of possible orientations in which an object can reach

a vacant location, provided the location is small enough. For a shape of a higher order of symmetry n_s , there is a greater number of possible orientations for deposition into a selective target on the lattice. Hence, the increase of the order of symmetry of the shape enhances the rate of single-particle adsorption. This is reflected in the fact that the adsorption of asymmetric shapes is slower than the adsorption of more regular and symmetric shapes.

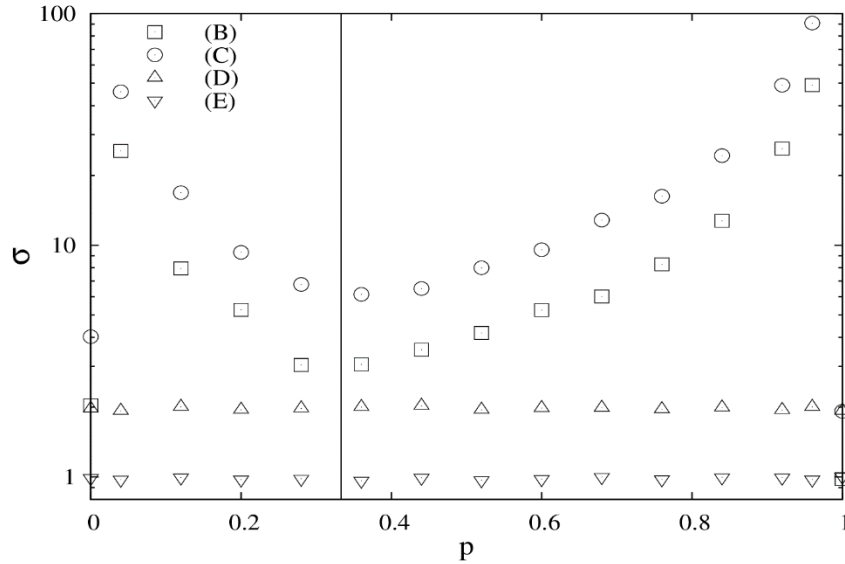


Figure 1. Dependence of the parameter σ [Eq. (1)] on probability p for shapes B, C, D, and E from Table I. The vertical line indicates the value of $p = 1/3$.

In the case of anisotropic deposition ($p \neq 1/3$), for all investigated shapes and all probabilities of adsorption in a horizontal direction, plots of $\ln[\theta_{jam} - \theta(t)]$ versus t are straight lines in the late times of the process. Analyzing the results for a large number of various shapes, we can see that the kinetics of anisotropic deposition is determined mainly by the symmetry properties of the object. For objects B, C, D and E (Table I), dependence of the parameter σ on the probability p is given in Fig. 1. For the k-mer B covering three lattice sites and for the angled object C, rapidity of the approach to the jamming limit is affected by the presence of anisotropy. The dependence of the parameter σ on the probability p is more prominent for the less symmetric object C. For the values of p close to zero, the deposition process is very slow. The relaxation time σ decreases with p , reaches a minimum for the isotropic case, and increases for higher values of p . For the less symmetric object C, $\sigma \simeq 4.0$ for $p = 0$, and $\sigma \simeq 2.0$ for $p = 1$. For $p = 1/3$, the expected result that $\sigma \simeq 6.0$ is obtained. Values of σ for the objects with symmetry axis of first order are twice higher than the corresponding values for the objects with symmetry axis of second order for each value of the probability p . Deposition of the objects with symmetry axis of third and sixth order is not affected by the presence of anisotropy. No matter what the value of the probability p is, $\sigma \simeq 2.0$ for the objects with symmetry axis of third order, and $\sigma \simeq 1.0$ for the objects with symmetry axis of sixth order.

As one can see from Fig. 2, the jamming coverage depends on the probability p for the shapes with symmetry axis of first and second order. On the contrary, for the objects with symmetry axis of third and sixth order, the values of θ_{jam} do not depend on p , and the isotropic values of

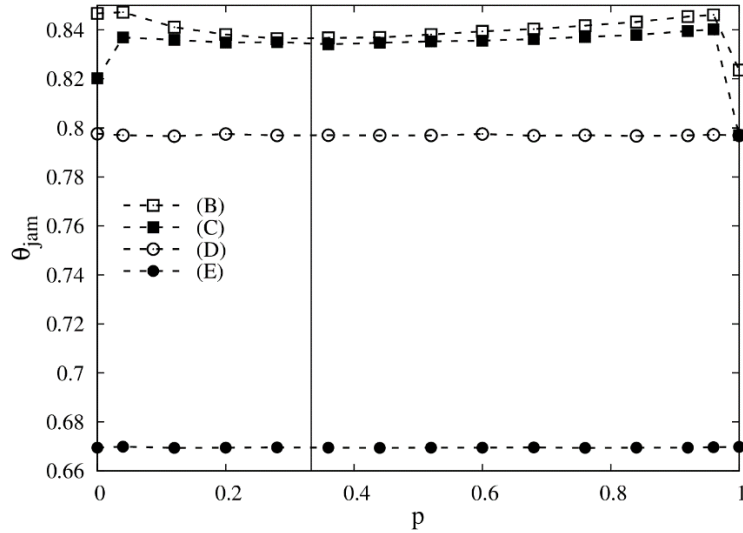


Figure 2. Dependence of the jamming coverage θ_{jam} on probability p for shapes B, C, D, and E from Table I. The vertical line indicates the value of $p = 1/3$.

jamming coverages are obtained [6]. At very early times of the process the depositing objects do not “feel” the presence of the already deposited ones and are placed randomly on to the lattice. However, in the late stages of deposition the objects must fit into small empty regions that favors the formation of clusters. Line segments and angled shapes deposited in the late stages of deposition must deposit parallel to the already deposited ones in order to avoid an intersection. This is reflected in the relatively high local packing of nearly parallel adsorbed objects in the vicinity of given object in the case of line segments and angled objects as compared to the triangles and hexagons. Such a different object view is the cause of the enhanced growth of very compact domains in the case of elongated shapes as compared to those in the case of more round (symmetric) shapes, resulting in a higher value of the jamming coverage fraction in the former case.

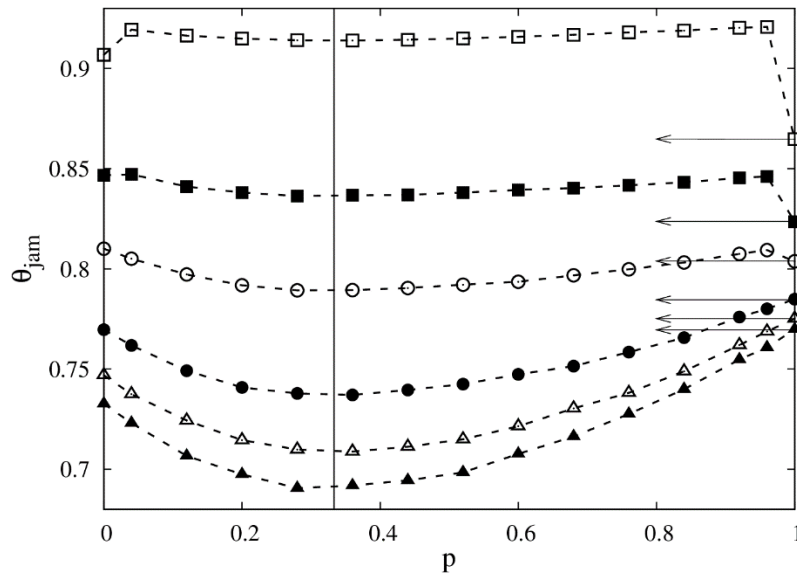


Figure 3. Dependence of the jamming coverage θ_{jam} on probability p for various k -mers.

The curves from top to bottom correspond to increasing values of $k = 2, 3, 4, 6, 8, 10$. The vertical line indicates the value of $p = 1/3$.

We also study the anisotropic RSA of k -mers. The simulations have been performed for line segments of lengths $l = 1, 2, \dots, 10$. For all investigated k -mers and for all probabilities p of

deposition in horizontal direction, plots of $\ln[\theta_{jam} - \theta(t)]$ versus t are straight lines for the late stages of deposition. Jamming coverage θ_{jam} also depends on the degree of anisotropy. From Fig.3 we can see that this dependence differs for k -mers of various lengths. For all objects, the jamming coverage θ_{jam} exhibits a local minimum near $p = 1/3$, i.e., for isotropic condition. For $k \geq 4$ this minimum is lower than the value of jamming coverage for deposition of k -mers in one dimension. However, the most striking feature is that a very small change in the probability p away from 0 or 1 brings an abrupt jump in the value of the jamming coverage θ_{jam} for the k -mers of small length ($k \leq 3$); e.g., when p changes from 0.96 to 1, the value of θ_{jam} for dimers drops from 0.92 to 0.86. The jump near $p = 0$ is smaller in magnitude.

Conclusion

We have investigated numerically the effect of anisotropy on the RSA of extended objects on a planar triangular lattice. A systematic approach is made by using the objects of different number of segments and rotational symmetries.

It was shown that the growth of the coverage $\theta(t)$ to the jamming limit θ_{jam} occurs via the exponential law (1), for all the shapes considered and for all values of probability p of deposition in a preferential direction. The simulations have shown that the kinetics of anisotropic deposition is determined mainly by the symmetry properties of the object. In the case of elongated and asymmetrical shapes, the relaxation time σ is found to increase with the degree of anisotropy. However, for rounded and symmetrical shapes, rapidity of the approach to the jamming state is not affected by the presence of anisotropy. A similar qualitative behavior of the jamming limit θ_{jam} in anisotropic condition is obtained; for highly symmetric objects, no dependence of the jamming coverage θ_{jam} on the probability p is observed within the statistical uncertainties. Nevertheless, the jamming coverage depends on the probability p for the shapes with lower-order symmetry axis.

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